

10/513699

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NEWS	1		Web Page for STN Seminar Schedule - N. America
NEWS	2	AUG 06	CAS REGISTRY enhanced with new experimental property tags
NEWS	3	AUG 06	FSTA enhanced with new thesaurus edition
NEWS	4	AUG 13	CA/CAPplus enhanced with additional kind codes for granted patents
NEWS	5	AUG 20	CA/CAPplus enhanced with CAS indexing in pre-1907 records
NEWS	6	AUG 27	Full-text patent databases enhanced with predefined patent family display formats from INPADOCDB
NEWS	7	AUG 27	USPATOLD now available on STN
NEWS	8	AUG 28	CAS REGISTRY enhanced with additional experimental spectral property data
NEWS	9	SEP 07	STN AnaVist, Version 2.0, now available with Derwent World Patents Index
NEWS	10	SEP 13	FORIS renamed to SOFIS
NEWS	11	SEP 13	INPADOCDB enhanced with monthly SDI frequency
NEWS	12	SEP 17	CA/CAPplus enhanced with printed CA page images from 1967-1998
NEWS	13	SEP 17	CAPplus coverage extended to include traditional medicine patents
NEWS	14	SEP 24	EMBASE, EMBAL, and LEMBASE reloaded with enhancements
NEWS	15	OCT 02	CA/CAPplus enhanced with pre-1907 records from Chemisches Zentralblatt
NEWS	16	OCT 19	BEILSTEIN updated with new compounds
NEWS	17	NOV 15	Derwent Indian patent publication number format enhanced
NEWS	18	NOV 19	WPIX enhanced with XML display format
NEWS	19	NOV 30	ICSD reloaded with enhancements
NEWS	20	DEC 04	LINPADOCDB now available on STN
NEWS	21	DEC 14	BEILSTEIN pricing structure to change
NEWS	22	DEC 17	USPATOLD added to additional database clusters
NEWS	23	DEC 17	IMSDRUGCONF removed from database clusters and STN
NEWS	24	DEC 17	DGENE now includes more than 10 million sequences
NEWS	25	DEC 17	TOXCENTER enhanced with 2008 MeSH vocabulary in MEDLINE segment
NEWS	26	DEC 17	MEDLINE and LMEDLINE updated with 2008 MeSH vocabulary
NEWS	27	DEC 17	CA/CAPplus enhanced with new custom IPC display formats
NEWS	28	DEC 17	STN Viewer enhanced with full-text patent content from USPATOLD
NEWS	29	JAN 02	STN pricing information for 2008 now available
NEWS	30	JAN 16	CAS patent coverage enhanced to include exemplified prophetic substances
NEWS	31	JAN 28	USPATFULL, USPAT2, and USPATOLD enhanced with new

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			custom IPC display formats
NEWS 32	JAN 28		MARPAT searching enhanced
NEWS 33	JAN 28		USGENE now provides USPTO sequence data within 3 days of publication
NEWS 34	JAN 28		TOXCENTER enhanced with reloaded MEDLINE segment
NEWS 35	JAN 28		MEDLINE and LMEDLINE reloaded with enhancements
NEWS EXPRESS		19 SEPTEMBER 2007:	CURRENT WINDOWS VERSION IS V8.2, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 19 SEPTEMBER 2007.
NEWS HOURS			STN Operating Hours Plus Help Desk Availability
NEWS LOGIN			Welcome Banner and News Items
NEWS IPC8			For general information regarding STN implementation of IPC 8

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FILE 'HOME' ENTERED AT 11:16:01 ON 01 FEB 2008

FILE 'REGISTRY' ENTERED AT 11:16:18 ON 01 FEB 2008
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STRUCTURE FILE UPDATES: 31 JAN 2008 HIGHEST RN 1001228-41-6
DICTIONARY FILE UPDATES: 31 JAN 2008 HIGHEST RN 1001228-41-6
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TSCA INFORMATION NOW CURRENT THROUGH June 29, 2007

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

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=>

Uploading C:\Program Files\Stnexp\Queries\10524517form3.str



chain nodes :
7 8 9 11 12 14 15 18 19 20 21
ring nodes :
1 2 3 4 5 6
ring/chain nodes :
16 24
chain bonds :
1-7 2-15 3-14 5-11 6-12 7-8 7-9 9-16 18-19 18-24 19-20 19-21
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds :
1-2 1-6 1-7 2-3 2-15 3-4 3-14 4-5 5-6 5-11 6-12 7-8 7-9 9-16 18-19
18-24 19-21
exact bonds :
19-20
isolated ring systems :
containing 1 :

G1:C,H,O,X

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 11:CLASS
12:CLASS 14:CLASS 15:CLASS 16:CLASS 18:CLASS 19:CLASS 20:CLASS 21:CLASS
24:CLASS

L1 STRUCTURE UPLOADED

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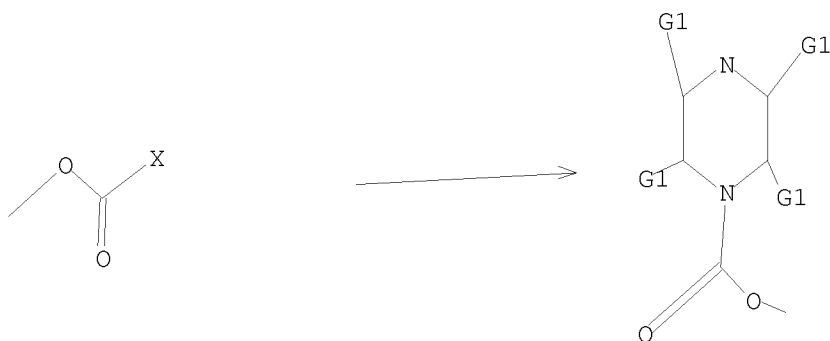
L1 HAS NO ANSWERS

L1 STR

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G1 C,H,O,X

Structure attributes must be viewed using STN Express query preparation.

=> s l1 full

FULL SEARCH INITIATED 11:16:51 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 96 TO ITERATE

100.0% PROCESSED 96 ITERATIONS

37 ANSWERS

SEARCH TIME: 00.00.01

L2 37 SEA SSS FUL L1

=> file caplus

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

178.36

178.57

FILE 'CAPLUS' ENTERED AT 11:16:56 ON 01 FEB 2008

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FILE COVERS 1907 - 1 Feb 2008 VOL 148 ISS 6

FILE LAST UPDATED: 31 Jan 2008 (20080131/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply. They are available for your review at:

<http://www.cas.org/infopolicy.html>

<12/04/2007>

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L3 17 L2

=> s 13 and py<2003

22927790 PY<2003

L4 17 L3 AND PY<2003

=> d ibib abs hitstr tot

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L4 ANSWER 1 OF 17 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2001:478090 CAPLUS

DOCUMENT NUMBER: 135:298146

TITLE: Dibasic inhibitors of human mast cell tryptase. Part 3: Identification of a series of potent and selective inhibitors containing the benzamidine functionality

AUTHOR(S): Dener, J. M.; Rice, K. D.; Newcomb, W. S.; Wang, V. R.; Young, W. B.; Gangloff, A. R.; Kuo, E. Y.-L.; Cregar, L.; Putnam, D.; Wong, M.

CORPORATE SOURCE: Departments of Medicinal Chemistry, Biochemistry, and Enzymology, Axys Pharmaceuticals, Inc., South San Francisco, CA, 94080, USA

SOURCE: Bioorganic & Medicinal Chemistry Letters (2001), 11(13), 1629-1633

CODEN: BMCLE8; ISSN: 0960-894X

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 135:298146

AB A survey of charged groups and linkers for a series of sym. and unsym. dibasic inhibitors is described, leading to several classes of potent and selective inhibitors. The inhibitors synthesized and tested were related to the known inhibitor APC-1390. In particular, the benzamidine functionality was identified as the most potent charged group investigated.

IT 178972-37-7

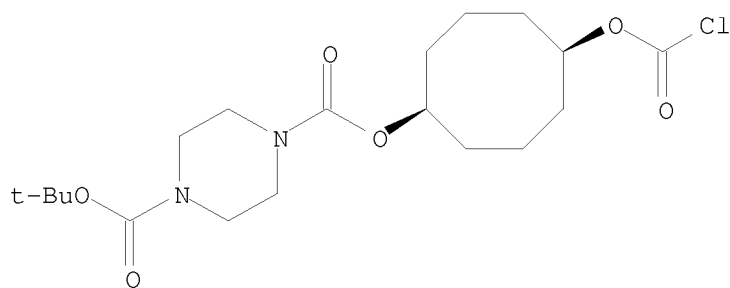
RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation and structure activity relationship of dibasic inhibitors of human mast cell tryptase related to APC-1390)

RN 178972-37-7 CAPLUS

CN 1,4-Piperazinedicarboxylic acid, cis-5-[(chlorocarbonyl)oxy]cyclooctyl 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Relative stereochemistry.



IT 202979-26-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

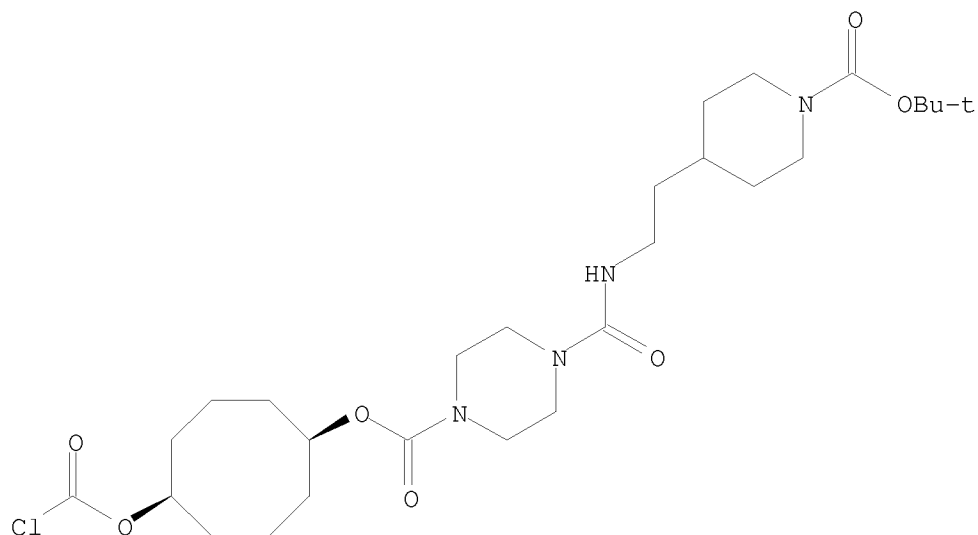
(preparation and structure activity relationship of dibasic inhibitors of human mast cell tryptase related to APC-1390)

RN 202979-26-8 CAPLUS

CN 1-Piperazinecarboxylic acid, 4-[[[2-[1-[(1,1-dimethylethoxy)carbonyl]-4-piperidinyl]ethyl]amino]carbonyl]-, cis-5-[(chlorocarbonyl)oxy]cyclooctyl ester (CA INDEX NAME)

10/513699

Relative stereochemistry.



REFERENCE COUNT:

13

THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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L4 ANSWER 2 OF 17 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2000:719714 CAPLUS

DOCUMENT NUMBER: 134:65802

TITLE: Dibasic inhibitors of human mast cell tryptase. Part 2: Structure-activity relationships and requirements for potent activity

AUTHOR(S): Rice, K. D.; Wang, V. R.; Gangloff, A. R.; Kuo, E. Y.-L.; Dener, J. M.; Newcomb, W. S.; Young, W. B.; Putnam, D.; Cregar, L.; Wong, M.; Simpson, P. J.

CORPORATE SOURCE: Exelixis Pharmaceuticals, Inc., South San Francisco, CA, 94080, USA

SOURCE: Bioorganic & Medicinal Chemistry Letters (2000), 10(20), 2361-2366

CODEN: BMCLE8; ISSN: 0960-894X

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Detailed structure-activity relationships (SARs) for a series of dibasic human tryptase inhibitors are presented. The structural requirements for potent inhibitory activity are remarkably broad with a range of core template modifications being well tolerated. Optimized inhibitors demonstrate potent anti-asthmatic activity in a sheep model of allergic asthma. APC-2059, a dibasic tryptase inhibitor with subnanomolar activity, has been advanced to phase II clin. trials for the treatment of both psoriasis and ulcerative colitis.

IT 178972-37-7P

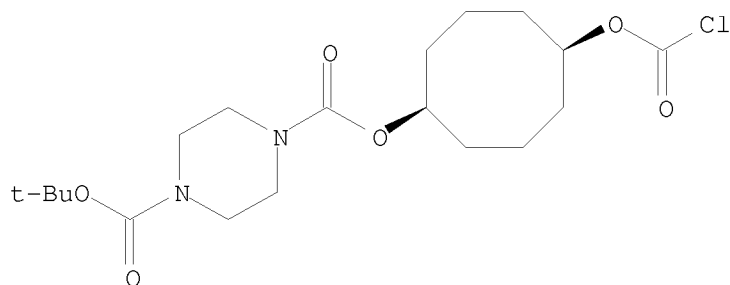
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(dibasic inhibitors of human mast cell tryptase and structure-activity relationships and requirements for potent activity as antiasthmatics)

RN 178972-37-7 CAPLUS

CN 1,4-Piperazinedicarboxylic acid, cis-5-[(chlorocarbonyl)oxy]cyclooctyl 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Relative stereochemistry.



REFERENCE COUNT: 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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L4 ANSWER 3 OF 17 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2000:96024 CAPLUS

DOCUMENT NUMBER: 132:137409

TITLE: Preparation of tryptase inhibitors

INVENTOR(S): Rice, Ken Duane; Dener, Jeffrey Mark; Gangloff, Anthony Robert; Kuo, Elaine Yee-lin

PATENT ASSIGNEE(S): AXYS Pharmaceuticals, Inc., USA

SOURCE: U.S., 27 pp., Cont.-in-part of U.S. Ser. No. 312,269, abandoned.

CODEN: USXXAM

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6022969	A	20000208	US 1995-522157	19950914 <--
CA 2200561	A1	19960328	CA 1995-2200561	19950914 <--
CN 1160398	A	19970924	CN 1995-195191	19950914 <--
HU 77770	A2	19980828	HU 1997-2059	19950914 <--
ZA 9508028	A	19960418	ZA 1995-8028	19950922 <--
IL 115405	A	20020725	IL 1995-115405	19950922 <--
HR 950499	B1	20030430	HR 1995-499	19950922
TW 442478	B	20010623	TW 1995-84110031	19950926 <--
LT 4234	B	19971027	LT 1997-65	19970410 <--
LV 11865	B	19980120	LV 1997-70	19970422 <--
US 6211228	B1	20010403	US 1999-280227	19990329 <--
PRIORITY APPLN. INFO.:			US 1994-312269	B2 19940923
			US 1995-522157	A3 19950914

OTHER SOURCE(S): MARPAT 132:137409

AB (ZX1X2X3X4X5)2Y [X1 = (oxa)alkylene, phenylene-interrupted alkylene, etc.; X2,X4 = CO, CO2, OCO2, CONH, etc.; X3 = alkylene, X9X10, X10X9, etc.; X5,X9 = alkylene; X10,Y = (hetero)cycloalkylene; Z = NH2, NHC(:NH)NH2, C(:NH)NH2] were prepared Thus, trans-cyclohexanedimethanol was bisesterified by OCNCH2CO2Et and the saponified product bisamidated by 4-(H2N)C6H4CH2NH2 to give, after NCNH2 N-acylation, Y[CH2O2CNHCH2CONHCH2C6H4[NHC(:NH)NH2]-4]2 (Y = trans-1,4-cyclohexylene). Data for biol. activity of title inhibitors were given.

IT 178972-37-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

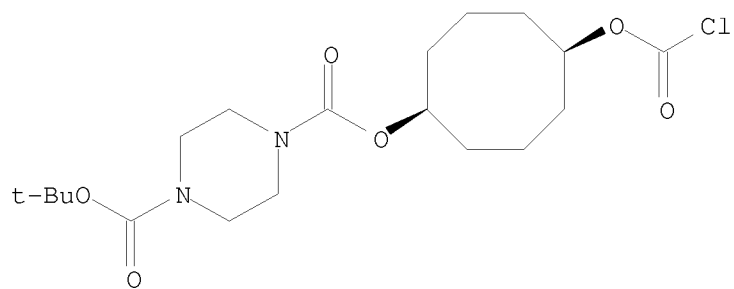
(preparation of tryptase inhibitors)

RN 178972-37-7 CAPLUS

CN 1,4-Piperazinedicarboxylic acid, cis-5-[(chlorocarbonyl)oxy]cyclooctyl 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Relative stereochemistry.

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REFERENCE COUNT:

27

THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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L4 ANSWER 4 OF 17 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1998:102855 CAPLUS

DOCUMENT NUMBER: 128:167443

TITLE: Novel compounds [cyclooctylene
bis(piperazinecarboxylates) and analogs] and
compositions for treating diseases associated with
tryptase activity

INVENTOR(S): Dener, Jeffrey Mark; Kuo, Elaine Yee-Lin; Rice, Ken
Duane; Wang, Vivian Rueywen; Young, Wendy Beth

PATENT ASSIGNEE(S): Arris Pharmaceutical Corporation, USA

SOURCE: PCT Int. Appl., 100 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

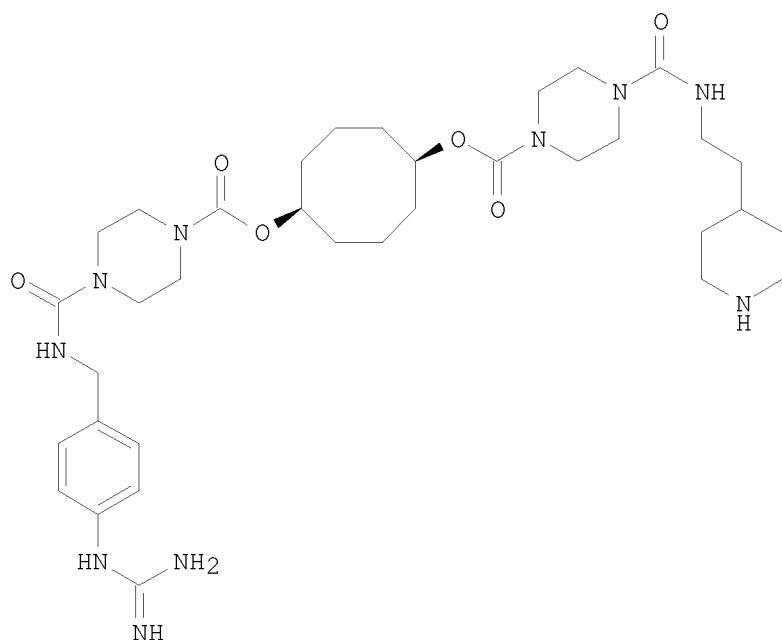
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

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WO 9804537	A1	19980205	WO 1997-US13422	19970730 <--
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW				
RW: GH, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
CA 2262542	A1	19980205	CA 1997-2262542	19970730 <--
AU 9739670	A	19980220	AU 1997-39670	19970730 <--
AU 733621	B2	20010517		
EP 934293	A1	19990811	EP 1997-937066	19970730 <--
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
CN 1226892	A	19990825	CN 1997-196877	19970730 <--
CN 1073103	B	20011017		
NZ 333713	A	20001222	NZ 1997-333713	19970730 <--
HU 2000003267	A2	20010628	HU 2000-3267	19970730 <--
HU 2000003267	A3	20020228		
JP 2001509787	T	20010724	JP 1998-509136	19970730 <--
FI 9900171	A	19990323	FI 1999-171	19990129 <--
NO 9900433	A	19990325	NO 1999-433	19990129 <--
KR 2000029679	A	20000525	KR 1999-700757	19990129 <--
LV 12291	B	20000420	LV 1999-27	19990218 <--
LT 4587	B	19991227	LT 1999-19	19990301 <--
LV 12458	B	20000920	LV 2000-30	20000225 <--
LV 12459	B	20000920	LV 2000-31	20000225 <--
PRIORITY APPLN. INFO.:			US 1996-23139P	P 19960730
			US 1997-895772	A 19970717
			WO 1997-US13422	W 19970730
			LV 1999-990027	A3 19990218
OTHER SOURCE(S):	MARPAT 128:167443			
GI				

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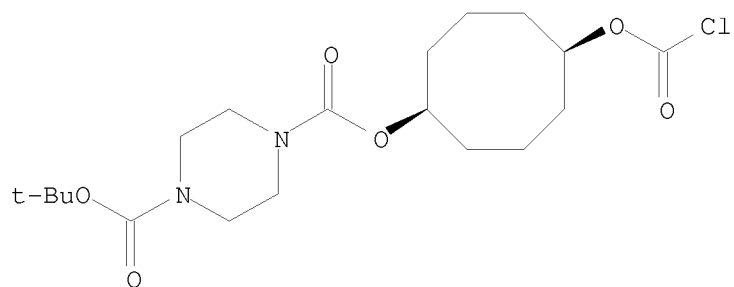


II

- AB The invention relates to novel compds. (R1X1X2X3X4)-X5-(X6X7X8X9R2) (I), which are tryptase inhibitors, and their pharmaceutically acceptable salts and N-oxides, as well as their uses as therapeutic agents, and methods of their preparation [wherein X5 = (hetero)cycloalkylene, (hetero)arylene; X4, X6 = bond, alkylene; X1, X9 = bond, CO, CO₂, OCO, CONR₃, NR₃CO, etc.; R₃ = H, alkyl, cycloalkyl; X3, X7 = CO, CO₂, OCO, CONR₃, NR₃CO, etc.; X2, X8 = (hetero)alkylene and/or cycloalkylene; R1 = amino, amidino, guanidino, certain N-heterocycles, etc., with optional (hetero)alkylene or other bridge; R2 = amino, 1-iminoethyl, methylamino, or certain N-heterocycles, with required or optional alkylene or other bridge]. The compds. are useful for treating a variety of conditions, including asthma, rheumatoid arthritis, and conjunctivitis. For instance, tert-Bu 4-[(4-guanidinobenzyl)carbamoyl]-1-piperazinecarboxylate trifluoroacetate underwent deprotection with CF₃CO₂H and amidation with cis-1,5-cyclooctylene chloroformate 4-(tert-butoxycarbonyl)-1-piperazinecarboxylate (77%), followed by a second deprotection and reaction with tert-Bu 4-(2-isocyanatoethyl)-1-piperidinecarboxylate, to give title compound II. Compds. I inhibited human tryptase in vitro with IC₅₀ in the range of 0.0001 to 41 μ M.
- IT 178972-37-7P 202979-21-3P 202979-26-8P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (intermediate; preparation of cyclooctylene bis(piperazinecarboxylates) and analogs as tryptase inhibitors)
- RN 178972-37-7 CAPLUS
- CN 1,4-Piperazinedicarboxylic acid, cis-5-[(chlorocarbonyl)oxy]cyclooctyl 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Relative stereochemistry.

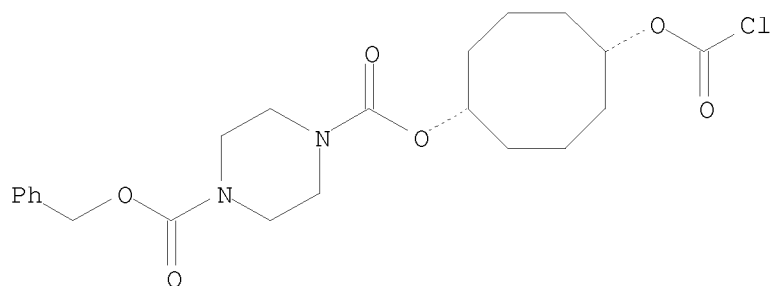
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RN 202979-21-3 CAPLUS

CN 1,4-Piperazinedicarboxylic acid, 5-[(chlorocarbonyl)oxy]cyclooctyl phenylmethyl ester, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.

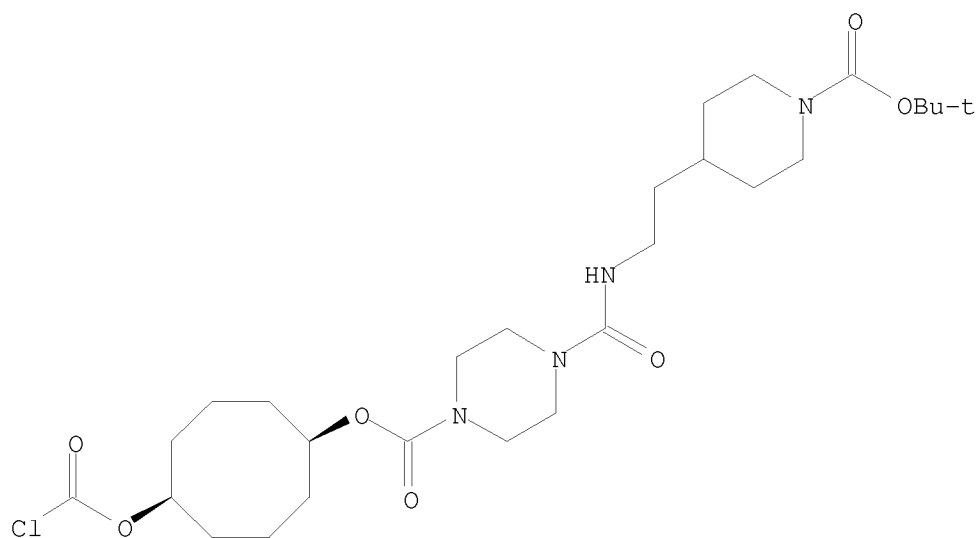


RN 202979-26-8 CAPLUS

CN 1-Piperazinecarboxylic acid, 4-[[[2-[1-[(1,1-dimethylethoxy)carbonyl]-4-piperidinyl]ethyl]amino]carbonyl]-, cis-5-[(chlorocarbonyl)oxy]cyclooctyl ester (CA INDEX NAME)

Relative stereochemistry.

10/513699



REFERENCE COUNT:

7

THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

<12/04/2007>

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L4 ANSWER 5 OF 17 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1996:446461 CAPLUS
 DOCUMENT NUMBER: 125:114691
 TITLE: Preparation of heterocyclic compound mast cell
 tryptase inhibitors
 INVENTOR(S): Rice, Ken D.; Dener, Jeffrey M.; Gangloff, Anthony R.;
 Kuo, Elaine Yee-lin
 PATENT ASSIGNEE(S): Arris Pharmaceutical Corporation, USA
 SOURCE: PCT Int. Appl., 87 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 2
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9609297	A1	19960328	WO 1995-US11814	19950914 <--
W: AU, BY, CA, CN, CZ, EE, FI, HU, JP, KR, LT, LV, MX, NO, NZ, PL, RU, SG, SI, SK, UA				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
CA 2200561	A1	19960328	CA 1995-2200561	19950914 <--
AU 9537180	A	19960409	AU 1995-37180	19950914 <--
AU 694275	B2	19980716		
EP 782571	A1	19970709	EP 1995-934993	19950914 <--
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
CN 1160398	A	19970924	CN 1995-195191	19950914 <--
JP 10506390	T	19980623	JP 1995-511002	19950914 <--
HU 77770	A2	19980828	HU 1997-2059	19950914 <--
RU 2159229	C2	20001120	RU 1997-106347	19950914 <--
EE 3525	B1	20011015	EE 1997-89	19950914 <--
PL 183552	B1	20020628	PL 1995-319587	19950914 <--
ZA 9508028	A	19960418	ZA 1995-8028	19950922 <--
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HR 950499	B1	20030430	HR 1995-499	19950922 <--
TW 442478	B	20010623	TW 1995-84110031	19950926 <--
FI 9701171	A	19970320	FI 1997-1171	19970320 <--
NO 9701305	A	19970506	NO 1997-1305	19970320 <--
NO 309605	B1	20010226		
LT 4234	B	19971027	LT 1997-65	19970410 <--
LV 11865	B	19980120	LV 1997-70	19970422 <--
PRIORITY APPLN. INFO.:			US 1994-312269	A 19940923
			WO 1995-US11814	W 19950914

OTHER SOURCE(S): MARPAT 125:114691

AB The title compds. (ZX1X2X3X4X5)2Y [I; Z = amino, guanidino, amidino; Y = (un)substituted cycloalkylene or heterocycloalkylene; X1 = (un)substituted alkylene, (un)substituted oxaalkylene; X2, X4 = CO, CO2, O2C, (un)substituted CONH, etc.; X3 = (un)substituted alkylene, etc.; X5 = (un)substituted alkylene], which are effective for the prevention and treatment of mast cell-mediated inflammatory disorders (e.g., asthma, arthritis, allergic rhinitis, etc.) via the inhibition of mast cell tryptase, are prepared and I-containing formulations claimed. Thus, cis-1,5-cyclooctylene bis[4-(4-guanidinophenylacetyl)-1-piperazinecarboxylate] was prepared and demonstrated a K_i of 0.00047 μM in a tryptase inhibition assay.

IT 178972-37-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

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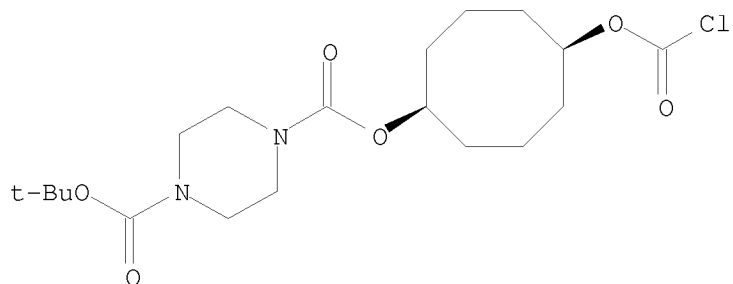
(Reactant or reagent)

(preparation of heterocyclic compound mast cell tryptase inhibitors)

RN 178972-37-7 CAPLUS

CN 1,4-Piperazinedicarboxylic acid, cis-5-[(chlorocarbonyl)oxy]cyclooctyl
1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Relative stereochemistry.



L4 ANSWER 6 OF 17 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1995:755182 CAPLUS

DOCUMENT NUMBER: 123:201656

TITLE: Thermoplastic graft copolymer elastomers with chain-folding or bifurcated side chains

AUTHOR(S): Eisenbach, Claus D.; Heinemann, Torsten

CORPORATE SOURCE: Bayreuther Inst. Makromol., Univ. Bayreuth, Bayreuth, D-95440, Germany

SOURCE: Macromolecular Chemistry and Physics (1995), 196(8), 2669-86

CODEN: MCHPES; ISSN: 1022-1352

PUBLISHER: Huethig & Wepf

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Graft copolymers with a poly(oxytetramethylene) main chain and mol. uniform oligourethane grafts were synthesized by substitution polycondensation of a telechelic polyether and the corresponding α, α' -bifunctional oligourethane macromonomer. The side chains were either characterized by a built-in constitutional unit allowing a sym. chain fold or by bifurcation with two equally long oligourethane branches. Differential scanning calorimetry, small-angle x-ray scattering, and dynamic mech. anal. proved a microphase-separated system with semicryst. oligourethane hard domains, and the materials were thermoplastic elastomers. These data and the comparative study of model compds. for the specially structured grafts and of poly(ether-urethane)s with sym. chain-folded segments illustrated that the morphol. and properties of these polyurethane elastomers could be perfectly mimicked by a graft copolymer with bifurcated side chains.

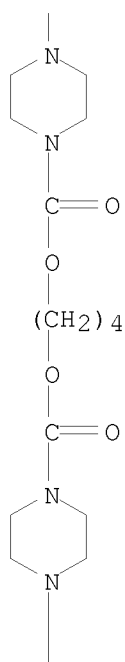
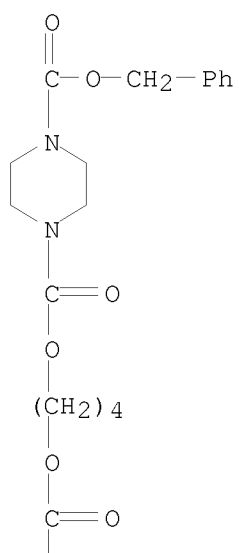
IT 162557-09-7

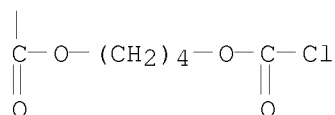
RL: RCT (Reactant); RACT (Reactant or reagent)

(condensation with piperazine-based urethane oligomer)

RN 162557-09-7 CAPLUS

CN 1,4-Piperazinedicarboxylic acid, 4-[[[4-[[4-[(chlorocarbonyl)oxy]butoxy]carbonyl]-1-piperazinyl]carbonyl]oxy]butyl 4-[[[4-[(phenylmethoxy)carbonyl]-1-piperazinyl]carbonyl]oxy]butyl ester (9CI) (CA INDEX NAME)





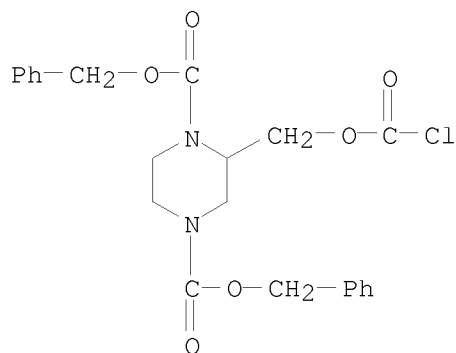
IT 161894-57-1

RL: RCT (Reactant); RACT (Reactant or reagent)

(condensation with piperazine-based urethane oligomers)

RN 161894-57-1 CAPLUS

CN 1,4-Piperazinedicarboxylic acid, 2-[[[(chlorocarbonyl)oxy]methyl]-, bis(phenylmethyl) ester (9CI) (CA INDEX NAME)



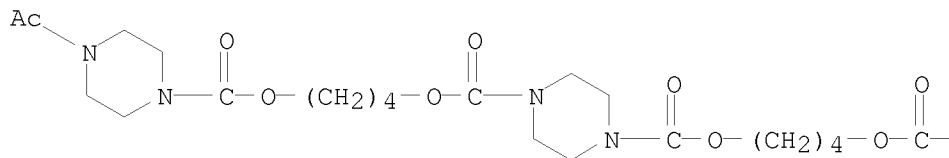
IT 167899-27-6P

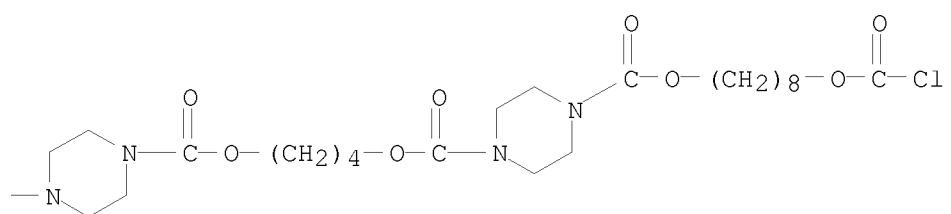
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and condensation with benzyl piperazinecarboxylate)

RN 167899-27-6 CAPLUS

CN 1,4-Piperazinedicarboxylic acid, 4-[[[4-[[4-[[4-(4-acetyl-1-piperazinyl)carbonyl]oxy]butoxy]carbonyl]-1-piperazinyl]carbonyl]oxy]butyl 4-[[[4-[[[8-[(chlorocarbonyl)oxy]octyl]oxy]carbonyl]-1-piperazinyl]carbonyl]oxy]butyl ester (9CI) (CA INDEX NAME)





L4 ANSWER 7 OF 17 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1995:629647 CAPLUS

DOCUMENT NUMBER: 123:10086

TITLE: Synthesis and Characterization of Graft Copolymers with Molecularly Uniform Urethane-Based Side Chains with Special Structural Elements

AUTHOR(S): Eisenbach, Claus D.; Heinemann, T.

CORPORATE SOURCE: Universitaet Bayreuth, Bayreuth, D-95440, Germany

SOURCE: Macromolecules (1995), 28(14), 4815-21

CODEN: MAMOBX; ISSN: 0024-9297

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Graft copolymers consisting of poly(oxytetramethylene) primary chain and distinctly engineered molecularly uniform oligo(N-alkylurethane) side chains with two constitutional units were synthesized and investigated by thermal and dynamic mech. anal. Microphase-separated systems with semicryst. oligourethane hard domains and characteristics of thermoplastic elastomers were observed for graft copolymers either with a spacer between the polyether backbone and the side chain or with specifically interacting graft end groups. The properties were correlated with contributions of special side-chain interactions and main chain-side chain coupling to the segregation and packing of the oligourethane branches.

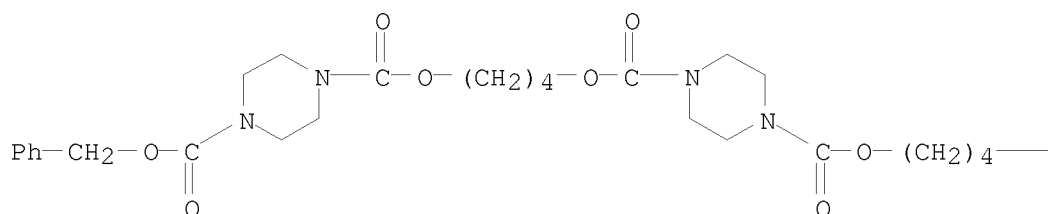
IT 124326-76-7

RL: RCT (Reactant); RACT (Reactant or reagent)
(condensation with functionalized piperazines)

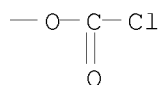
RN 124326-76-7 CAPLUS

CN 1,4-Piperazinedicarboxylic acid, 4-[[[4-[[4-[(chlorocarbonyl)oxy]butoxy]carbonyl]-1-piperazinyl]carbonyl]oxy]butyl phenylmethyl ester (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 1-B



IT 161894-57-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

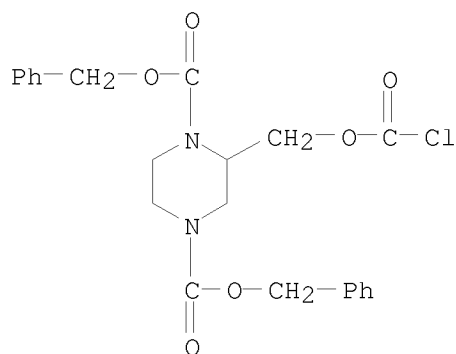
10/513699

(Reactant or reagent)

(preparation and condensation with methylaminoalkanols)

RN 161894-57-1 CAPLUS

CN 1,4-Piperazinedicarboxylic acid, 2-[[[(chlorocarbonyl)oxy]methyl]-, bis(phenylmethyl) ester (9CI) (CA INDEX NAME)



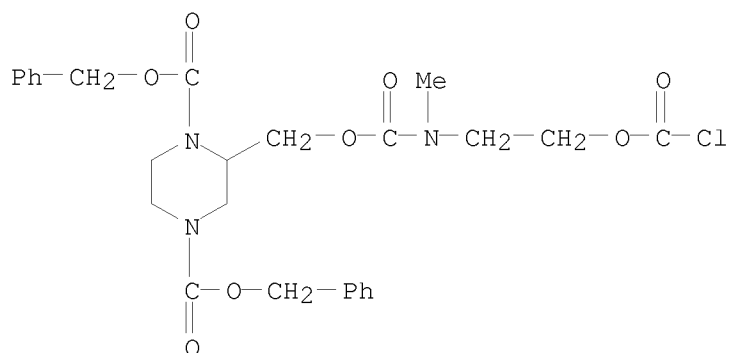
IT 163361-18-0P 163361-19-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and condensation with oligomeric polyurethanes)

RN 163361-18-0 CAPLUS

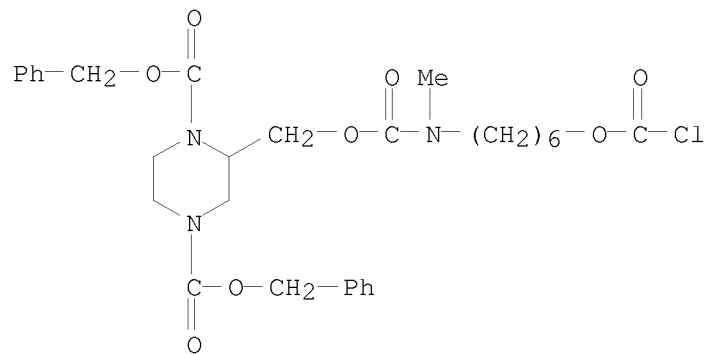
CN 1,4-Piperazinedicarboxylic acid, 2-[[[[[2-[(chlorocarbonyl)oxy]ethyl]methylamino]carbonyl]oxy]methyl]-, bis(phenylmethyl) ester (9CI) (CA INDEX NAME)



RN 163361-19-1 CAPLUS

CN 1,4-Piperazinedicarboxylic acid, 2-[[[[[6-[(chlorocarbonyl)oxy]hexyl]methylamino]carbonyl]oxy]methyl]-, bis(phenylmethyl) ester (9CI) (CA INDEX NAME)

10/513699



<12/04/2007>

Erich Leese

10/513699

L4 ANSWER 8 OF 17 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1995:613893 CAPLUS

DOCUMENT NUMBER: 123:35049

TITLE: Synthesis and properties of segmented poly(ether-urethanes) with specially designed and symmetrically chain-folding poly(N-alkylurethane) hard segments

AUTHOR(S): Eisenbach, Claus D.; Stadler, Edmund

CORPORATE SOURCE: Makromolekulare Chemie II, Universitaet Bayreuth, Bayreuth, D-95440, Germany

SOURCE: Macromolecular Chemistry and Physics (1995), 196(6), 1981-97

CODEN: MCHPES; ISSN: 1022-1352

PUBLISHER: Huethig & Wepf

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The study of a series of elastomeric segmented poly(ether urethanes) with highly flexible poly(oxytetramethylene) soft segments and especially designed, molecularly uniform poly(N-alkylurethane) hard segments based on piperazine and 1,4-butanediol bischloroformate has shown that size, shape and perfection of the hard domains can be varied by both the primary structure of the urethane chain and the sample history. Depending on the conformation or the stereogeometry of the built-in central constitutive hard segment unit, chain-extended or chain-folded hard segment crystallization, i.e., the formation of cylindrical or lamellar shaped hard domains can be achieved. These thermoplastic elastomers exhibit distinctly different properties which correlate systematically with the supermol. structure and the corresponding hard segment architecture, resp.

IT 164396-90-1P 164396-92-3P 164396-94-5P

164396-96-7P 164396-98-9P 164397-00-6P

164397-02-8P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)

(preparation and properties of elastomeric segmented polyether-polyurethanes with specially designed and sym. chain-folding poly(N-alkylurethane) hard segments)

RN 164396-90-1 CAPLUS

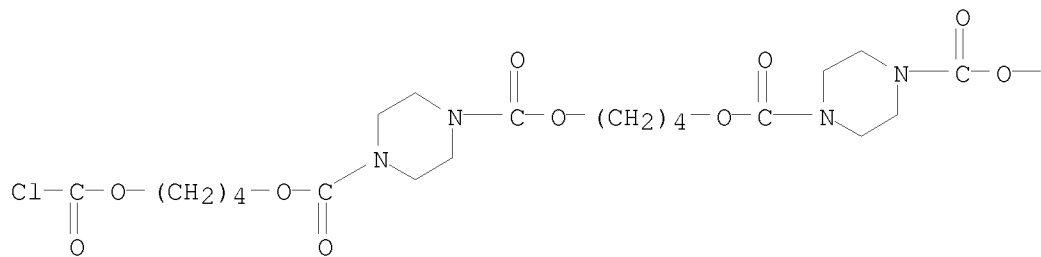
CN 1,4-Piperazinedicarboxylic acid, 1,4-butanediyl bis[4-[[[4-[[4-[(chlorocarbonyl)oxy]butoxy]carbonyl]-1-piperazinyl]carbonyl]oxy]butyl] ester, polymer with α -(1-piperazinylcarbonyl)- ω -[(1-piperazinylcarbonyl)oxy]poly(oxy-1,2-ethanediyl), block (9CI) (CA INDEX NAME)

CM 1

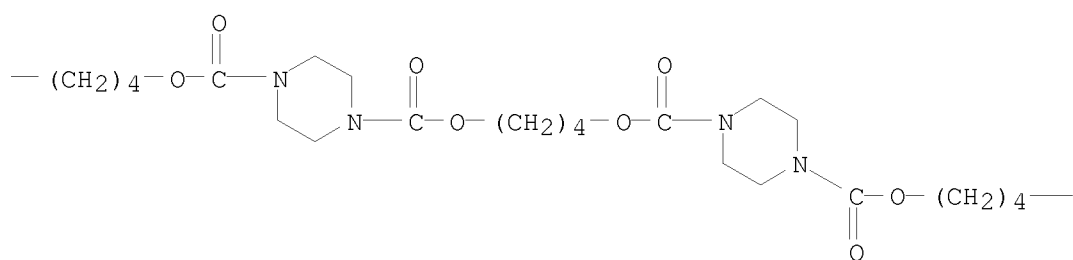
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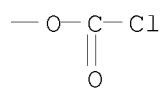
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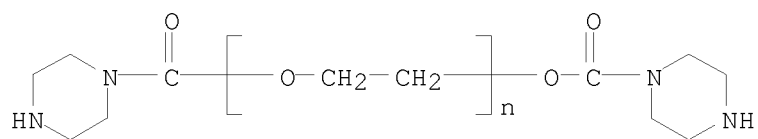


CM 2

CRN 133626-36-5

CMF (C2 H4 O)_n C10 H18 N4 O3

CCI PMS



RN 164396-92-3 CAPLUS

10/513699

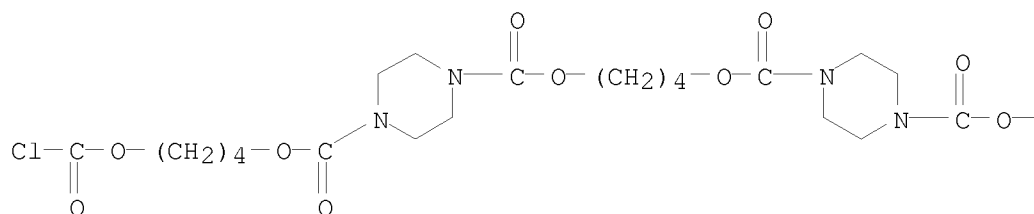
CN 1,4-Piperazinedicarboxylic acid, 1,6-hexanediyl bis[4-[[[4-[[4-[(chlorocarbonyl)oxy]butoxy]carbonyl]-1-piperazinyl]carbonyl]oxy]butyl] ester, polymer with α -(1-piperazinylcarbonyl)- ω -[(1-piperazinylcarbonyl)oxy]poly(oxy-1,2-ethanediyl), block (9CI) (CA INDEX NAME)

CM 1

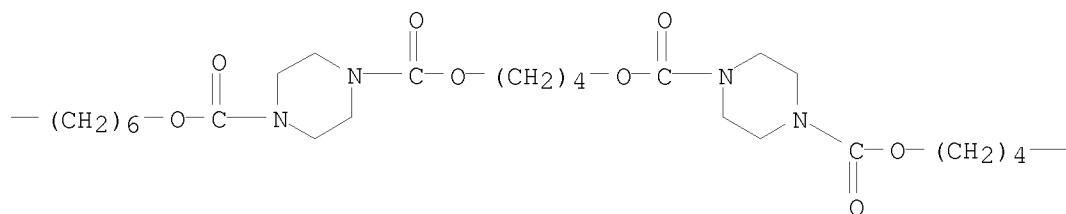
CRN 164396-91-2

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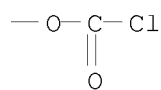
PAGE 1-A



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PAGE 1-C



CM 2

CRN 133626-36-5

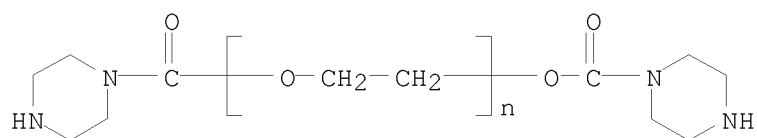
CMF (C2 H4 O)_n C10 H18 N4 O3

CCI PMS

<12/04/2007>

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10/513699



RN 164396-94-5 CAPLUS

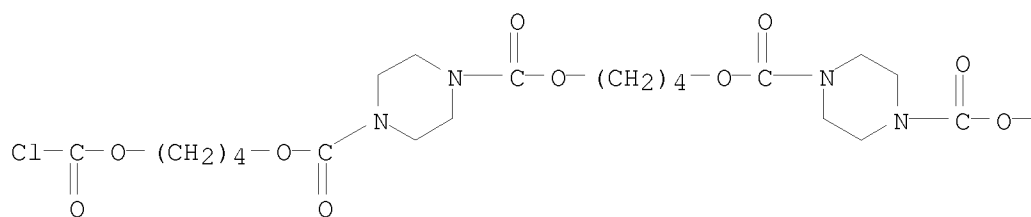
CN 1,4-Piperazinedicarboxylic acid, 1,8-octanediyl bis[4-[[[4-[[4-[(chlorocarbonyl)oxy]butoxy]carbonyl]-1-piperazinyl]carbonyl]oxy]butyl] ester, polymer with α -(1-piperazinylcarbonyl)- ω -[(1-piperazinylcarbonyl)oxy]poly(oxy-1,2-ethanediyl), block (9CI) (CA INDEX NAME)

CM 1

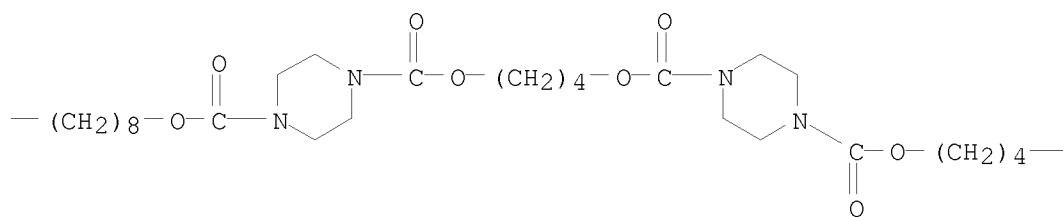
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CMF C50 H80 Cl2 N8 O20

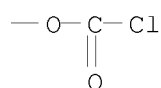
PAGE 1-A



PAGE 1-B



PAGE 1-C



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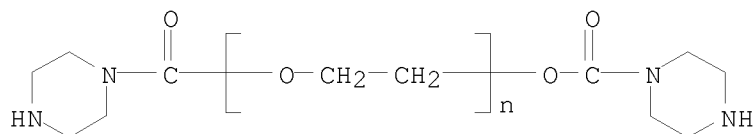
10/513699

CM 2

CRN 133626-36-5

CMF (C2 H4 O)_n C10 H18 N4 O3

CCI PMS



RN 164396-96-7 CAPLUS

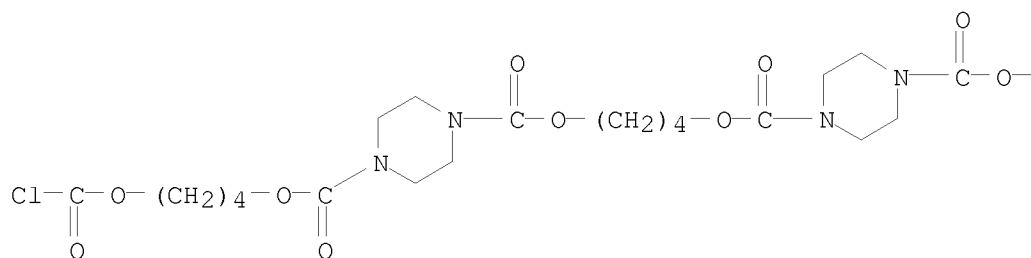
CN 1,4-Piperazinedicarboxylic acid, 1,4-butanediyl bis[4-[[[4-[[[4-[[4-[(chlorocarbonyl)oxy]butoxy]carbonyl]-1-piperazinyl]carbonyl]oxy]butoxy]carbonyl]-1-piperazinyl]carbonyl]oxy]butyl] ester, polymer with α -(1-piperazinylcarbonyl)- ω -[(1-piperazinylcarbonyl)oxy]poly(oxy-1,2-ethanediyl), block (9CI) (CA INDEX NAME)

CM 1

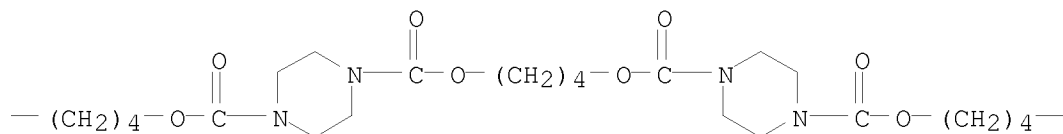
CRN 164396-95-6

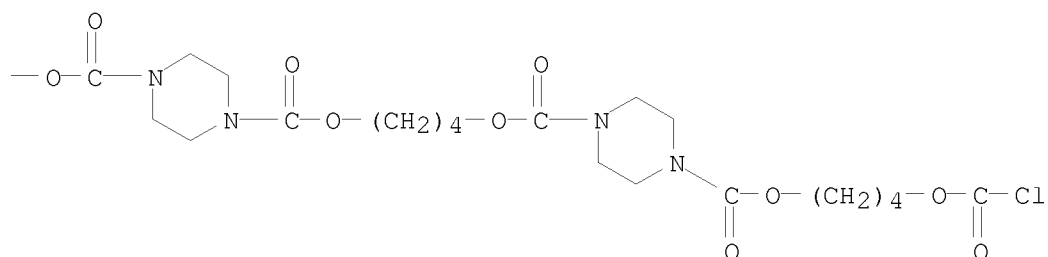
CMF C66 H104 Cl2 N12 O28

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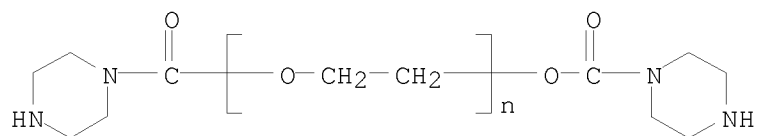


CM 2

CRN 133626-36-5

CMF (C2 H4 O)_n C10 H18 N4 O3

CCI PMS



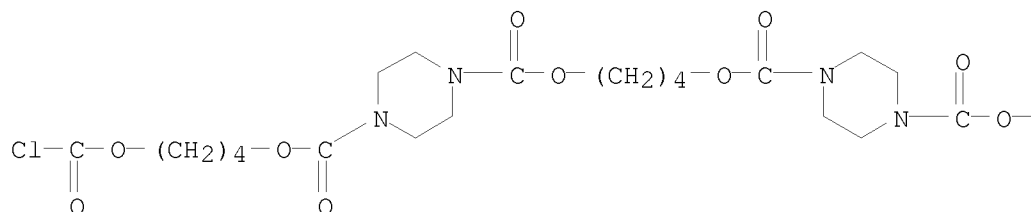
RN 164396-98-9 CAPLUS

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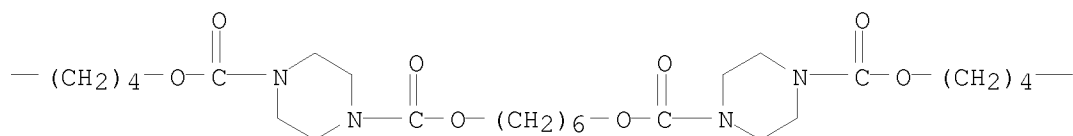
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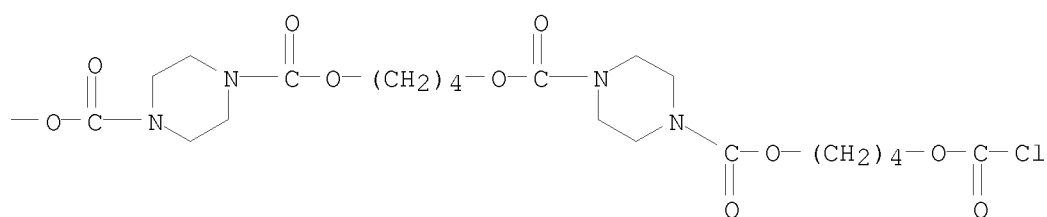
CMF C68 H108 C12 N12 O28



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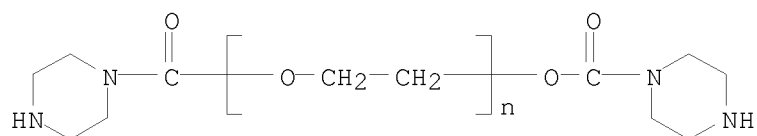


CM 2

CRN 133626-36-5

CMF (C2 H4 O)_n C10 H18 N4 O3

CCI PMS



RN 164397-00-6 CAPLUS

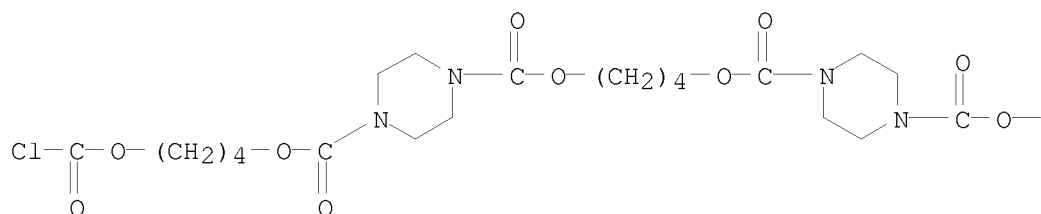
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 rbonyl]-1-piperazinyl]carbonyl]oxy]butyl] ester, polymer with
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 xy-1,2-ethanediyl) (9CI) (CA INDEX NAME)

CM 1

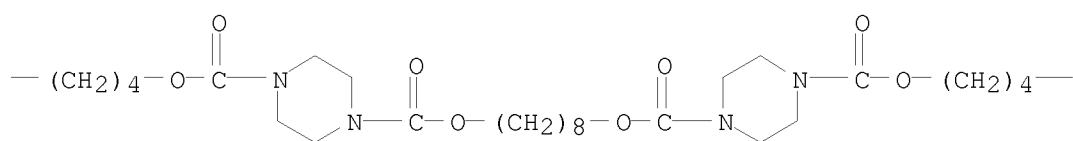
CRN 164396-99-0

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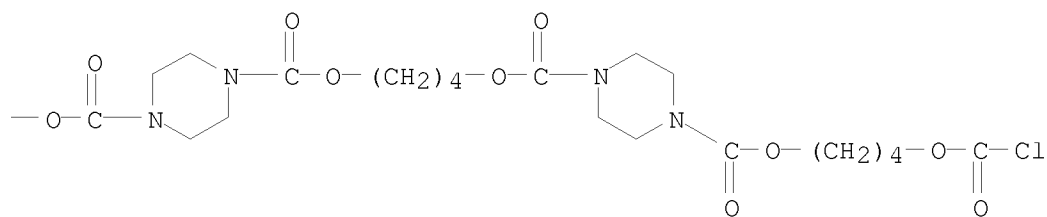
PAGE 1-A



PAGE 1-B



PAGE 1-C

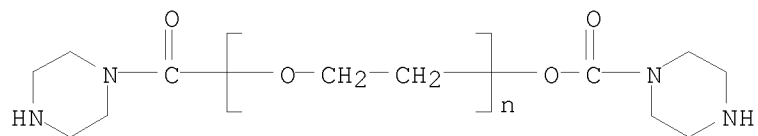


CM 2

CRN 133626-36-5

CMF (C2 H4 O)_n C10 H18 N4 O3

CCI PMS



RN 164397-02-8 CAPLUS

CN 1,4-Piperazinedicarboxylic acid, 1,2-phenylenebis(oxy-2,1-ethanediyl)
 bis[4-[[[4-[[[4-[[[4-[(chlorocarbonyl)oxy]butoxy]carbonyl]-1-
 piperazinyl]carbonyl]oxy]butoxy]carbonyl]-1-piperazinyl]carbonyl]oxy]butyl
] ester, polymer with α-(1-piperazinylcarbonyl)-ω-[(1-

10/513699

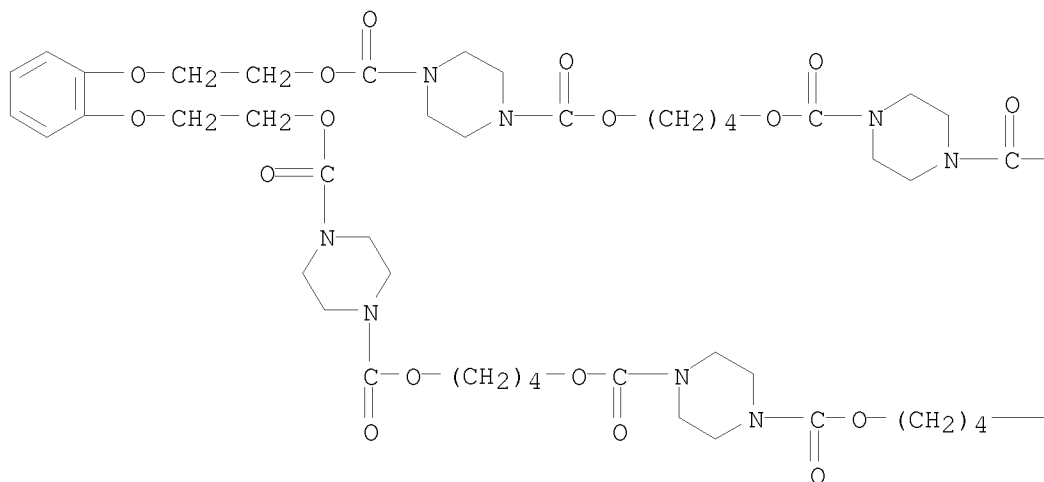
piperazinyldicarbonyloxy]poly(oxy-1,2-ethanediyl), block (9CI) (CA INDEX NAME)

CM 1

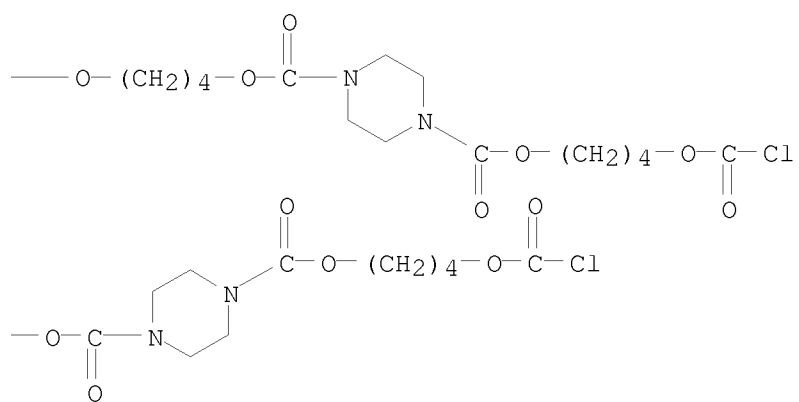
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CMF C72 H108 Cl2 N12 O30

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CM 2

CRN 133626-36-5

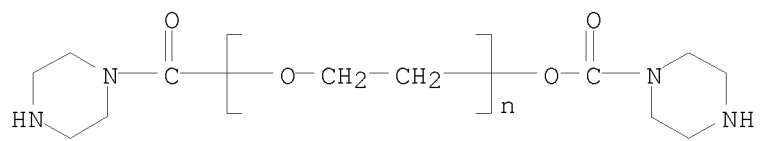
CMF (C2 H4 O)_n Cl10 H18 N4 O3

<12/04/2007>

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10/513699

CCI PMS



<12/04/2007>

Erich Leese

L4 ANSWER 9 OF 17 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1995:470956 CAPLUS

DOCUMENT NUMBER: 122:240500

TITLE: Synthesis and properties of molecularly uniform oligourethanes with chain-folding units in the center

AUTHOR(S): Eisenbach, Claus D.; Stadler, Edmund; Enkelmann, Volker

CORPORATE SOURCE: Univ. Bayreuth, Bayreuth, D-95440, Germany

SOURCE: Macromolecular Chemistry and Physics (1995), 196(3), 833-56

CODEN: MCHPES; ISSN: 1022-1352

PUBLISHER: Huethig & Wepf

DOCUMENT TYPE: Journal

LANGUAGE: English

AB A series of molecularly uniform poly(N-alkylurethanes) with a systematically varied and tailored chain architecture has been synthesized. The packing and superstructure can be controlled by the primary structure of the urethane chain and reversibly altered by the sample treatment, resp. Depending on the conformation or the stereogeometry of the constitutive unit built in the middle of the oligourethane, chain-extended or chain-folded crystallization of the urethane chain can occur. The packing order, i.e., adjacent reentry chain-folding or chain-extended crystallization, and the thermal properties of the oligourethanes are related to the chemical structure of the central constitutive unit.

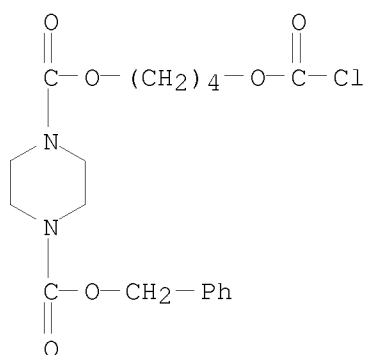
IT 25539-29-1P, Benzyl 4-chloroformyloxybutyl 1,4-piperazinedicarboxylate 124326-76-7P 162557-09-7P 162557-10-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(intermediates of molecularly uniform oligourethanes with chain-folding units in the center)

RN 25539-29-1 CAPLUS

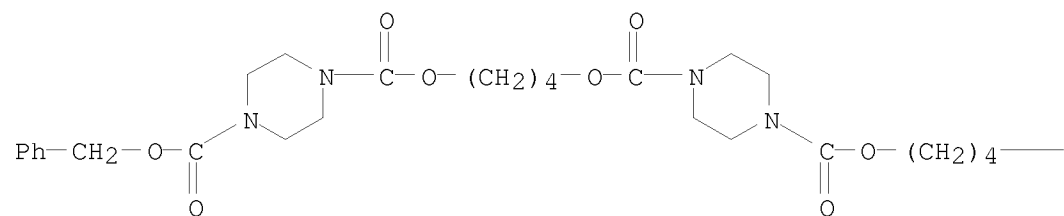
CN 1,4-Piperazinedicarboxylic acid, 4-[(chlorocarbonyl)oxy]butyl phenylmethyl ester (9CI) (CA INDEX NAME)



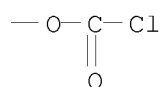
RN 124326-76-7 CAPLUS

CN 1,4-Piperazinedicarboxylic acid, 4-[[[4-[[4-[(chlorocarbonyl)oxy]butoxy]carbonyl]-1-piperazinyl]carbonyl]oxy]butyl phenylmethyl ester (9CI) (CA INDEX NAME)

PAGE 1-A



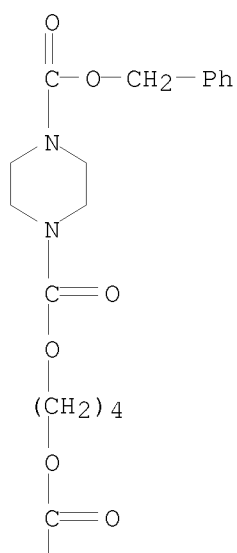
PAGE 1-B

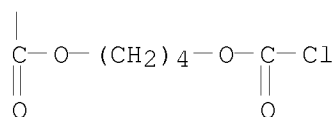
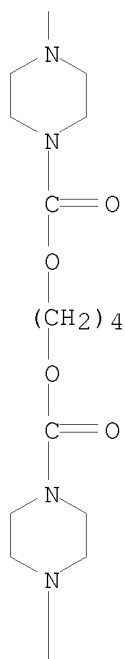


RN 162557-09-7 CAPLUS

CN 1,4-Piperazinedicarboxylic acid, 4-[[[4-[[4-[(chlorocarbonyl)oxy]butoxy]carbonyl]-1-piperazinyl]carbonyl]oxy]butyl 4-[[[4-[(phenylmethoxy)carbonyl]-1-piperazinyl]carbonyl]oxy]butyl ester (9CI) (CA INDEX NAME)

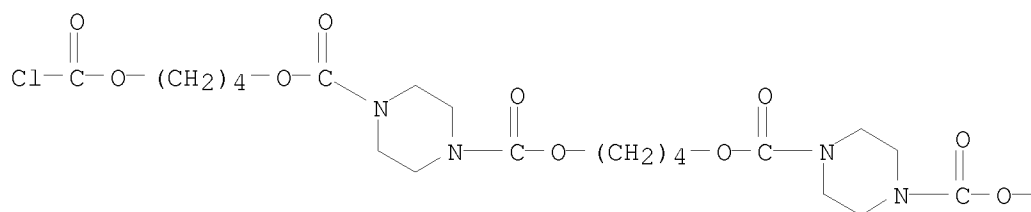
PAGE 1-A

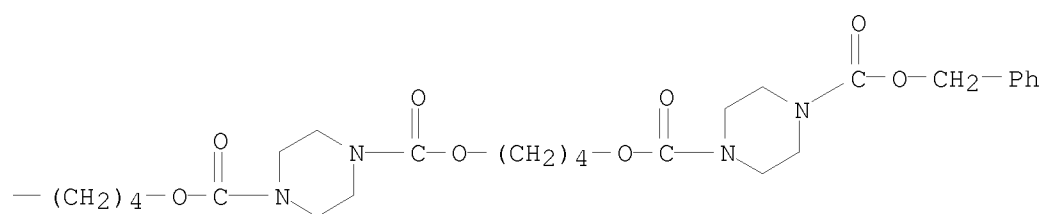




RN 162557-10-0 CAPLUS

CN 1,4-Piperazinedicarboxylic acid, 4-[[[4-[[4-[[[4-[[4-
 [(chlorocarbonyl)oxy]butoxy]carbonyl]-1-piperazinyl]carbonyl]oxy]butoxy]ca
 rbonyl]-1-piperazinyl]carbonyl]oxy]butyl 4-[[[4-[(phenylmethoxy)carbonyl]-
 1-piperazinyl]carbonyl]oxy]butyl ester (9CI) (CA INDEX NAME)





L4 ANSWER 10 OF 17 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1995:433747 CAPLUS

DOCUMENT NUMBER: 122:190010

TITLE: Synthesis and Characterization of Thermoplastic Graft Copolymer Elastomers with a Polyether Main Chain and Uniform Urethane-Based Side Chains

AUTHOR(S): Eisenbach, Claus D.; Heinemann, T.

CORPORATE SOURCE: Universitaet Bayreuth, Bayreuth, D-95440, Germany

SOURCE: Macromolecules (1995), 28(7), 2133-9

CODEN: MAMOBX; ISSN: 0024-9297

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The polycondensation reaction of molecularly uniform α, α' -bifunctional oligourethane macromonomers with α -(chlorocarbonyl)- ω -(chloroformyl)poly(oxytetramethylene) yielded graft copolymers with an exactly defined primary structure, i.e., with known graft distribution and length; corresponding oligomeric model compds. were also obtained from the macromonomers by reaction with a monofunctional chain extender. Above a certain length of the side chains the graft copolymers exhibited the typical properties of thermoplastic elastomers. A microphase-separated system was formed in which the grafts have segregated to form semicryst. hard domains dispersed in a continuous polyether soft phase. The study of the thermal and mech. properties of these thermoplastic graft copolymer elastomers and their model compds. in comparison with analogously built segmented poly(ether-urethanes) revealed a specific influence of the branching on the packing of the polyurethane grafts and comparable systematics in the elastomer properties with the number of repeat units in the polyurethane graft.

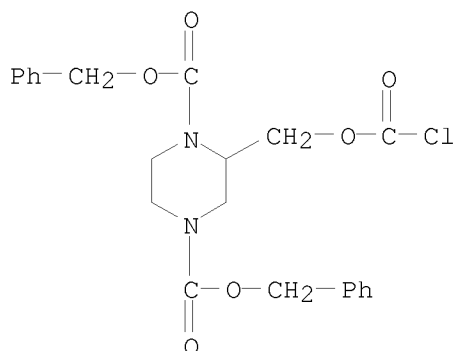
IT 161894-57-1, Dibenzyl 2-[[[(chloroformyl)oxy]methyl]-N,N'-piperazine dicarboxylate

RL: RCT (Reactant); RACT (Reactant or reagent)

(synthesis and characterization of thermoplastic graft copolymer elastomers with a polyether main chain and uniform urethane-based side chains)

RN 161894-57-1 CAPLUS

CN 1,4-Piperazinedicarboxylic acid, 2-[[[(chlorocarbonyl)oxy]methyl]-, bis(phenylmethyl) ester (9CI) (CA INDEX NAME)



L4 ANSWER 11 OF 17 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1994:632829 CAPLUS

DOCUMENT NUMBER: 121:232829

TITLE: Structure of the hard segments in non hydrogen bond forming polyurethane elastomers as derived from oligomeric model compounds

AUTHOR(S): Eisenbach, Claus D.; Nefzger, Hartmut; Hayen, Heidi

CORPORATE SOURCE: Makromolekulare Chemie II, Universitat Bayreuth, Bayreuth, D-95440, Germany

SOURCE: Macromolecular Chemistry and Physics (1994), 195(10), 3325-42

CODEN: MCHPES; ISSN: 1022-1352

DOCUMENT TYPE: Journal

LANGUAGE: English

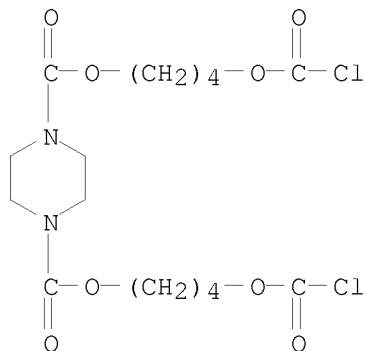
AB Several molecularly uniform oligourethane model compds. for the hard segment of segmented polyurethane elastomers with piperazine- (PIP) and tetramethylene bischloroformate-based hard segments have been synthesized. X-ray structure anal. was performed on single crystals with both compds. representing different parts of the piperazine-1,4-diylcarbonyloxytetramethyleneoxycarbonyl repeating unit or containing ≥ 1 complete repeating unit and methylurethane end groups. A common feature of the model compds. investigated was that the PIP rings are in the chair conformation; the oxytetramethyleneoxy unit is in the g+tg- conformation, which is also the conformation of the higher melting modification of the 2 hard-segment model polymorphs. The conformation and packing model of the hard segment was derived from the crystal structure of the model compound containing 1 repeating unit by connecting the 2 Me end groups of successive mols. by a CH₂CH₂ unit without shifting the mols., i.e., by replacement of 2 opposing OMe groups by an oxytetramethyleneoxy chain in the g+tg- conformation. The resulting cell for the polyurethane model structure is triclinic and contains 2 units of half a polymer repeat, and is in excellent agreement with the exptl. X-ray powder diffraction pattern of the hard-segment polymer.

IT 158533-85-8P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(in preparation of model compds. for structural study of urethane rubber with hard segments without forming hydrogen bonding)

RN 158533-85-8 CAPLUS

CN 1,4-Piperazinedicarboxylic acid, bis[4-[(chlorocarbonyl)oxy]butyl] ester
(9CI) (CA INDEX NAME)



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<12/04/2007>

Erich Leese

L4 ANSWER 12 OF 17 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1991:493285 CAPLUS

DOCUMENT NUMBER: 115:93285

TITLE: Deuteron NMR measurements of order and mobility in the hard segments of a model polyurethane

AUTHOR(S): Kornfield, J. A.; Spiess, H. W.; Nefzger, H.; Hayen, H.; Eisenbach, C. D.

CORPORATE SOURCE: Max-Planck-Inst. Polymerforsch., Mainz, D-6500, Germany

SOURCE: Macromolecules (1991), 24(17), 4787-95

CODEN: MAMOBX; ISSN: 0024-9297

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Pulsed deuteron NMR results are reported for a series of segmented model polyurethanes with monodisperse hard segments containing specifically labeled sites. The hard segments consist of 5 piperazine rings separated by carbonyloxytetramethyleneoxycarbonyl spacers. The soft segments are polydisperse poly(tetramethylene oxide). The results indicate that 85% of the hard segments exist in the hard phase, with low mobility <410 K. The rest of the hard segments are dispersed in the soft phase, with high mobility >260 K. Mol. mobility is much greater at the exterior than the center of hard segments in the hard phase at 300-410 K.

IT 124326-76-7P

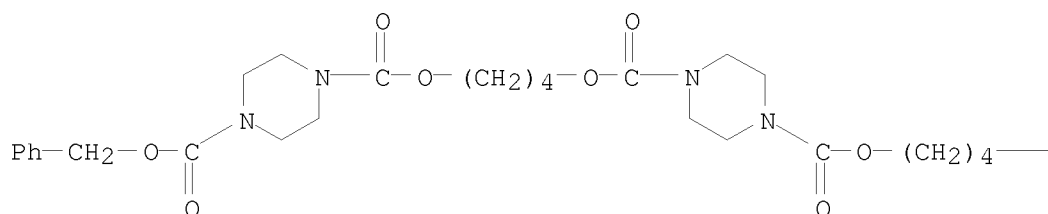
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and reaction of, with piperazine)

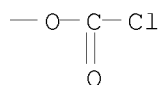
RN 124326-76-7 CAPLUS

CN 1,4-Piperazinedicarboxylic acid, 4-[[[4-[[4-[(chlorocarbonyl)oxy]butoxy]carbonyl]-1-piperazinyl]carbonyl]oxy]butyl phenylmethyl ester (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 1-B



IT 25539-29-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

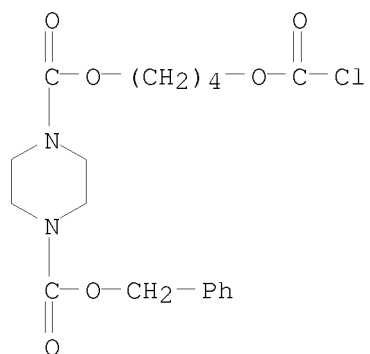
10/513699

(Reactant or reagent)

(preparation and reaction of, with tert-butoxybutyl piperazinecarboxylate)

RN 25539-29-1 CAPLUS

CN 1,4-Piperazinedicarboxylic acid, 4-[(chlorocarbonyl)oxy]butyl phenylmethyl
ester (9CI) (CA INDEX NAME)



L4 ANSWER 13 OF 17 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1990:22161 CAPLUS

DOCUMENT NUMBER: 112:22161

TITLE: Control of self-organization and structure of macromolecules through built-in joints

AUTHOR(S): Eisenbach, Claus D.; Hayen, Heidi; Nefzger, Hartmut

CORPORATE SOURCE: Univ. Bayreuth, Bayreuth, D-8580, Fed. Rep. Ger.

SOURCE: Makromolekulare Chemie, Rapid Communications (1989), 10(9), 463-75

CODEN: MCRCD4; ISSN: 0173-2803

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Crystallizable oligourethanes and polyurethanes were prepared from piperazine and derivs., tetramethylene bis(chloroformate), and hexamethylene bis(chloroformate) (which acted as a flexible joint), and crystallization and dynamic mech. properties were studied. MeOCOZ(COO(CH₂)₄COZ)7COOMe (I) and MeOCOZ(COO(CH₂)₄COZ)3COO(CH₂)₆COZ(COO(CH₂)₄COZ)3COOMe (II) where Z = 1,4-piperazinediyl were synthesized. When the center unit was rigid tetramethylene as in I the chains crystallized in extended configuration; when the center unit was flexible hexamethylene as in II the chains crystallized in both extended and folded configurations. DSC showed 1 sharp endotherm from the melting of extended-chain crystals in I but showed 2 endotherms from the melting of extended-chain crystals and folded-chain crystals in II. Dynamic mech. measurements showed that polyurethanes which contained a central hexamethylene unit softened at a much lower temperature, corresponding to the melting of folded-chain crystals, than those which contained a central tetramethylene unit.

IT 25539-29-1P, Benzyl 4-chloroformyloxybutyl piperazine-1,4-

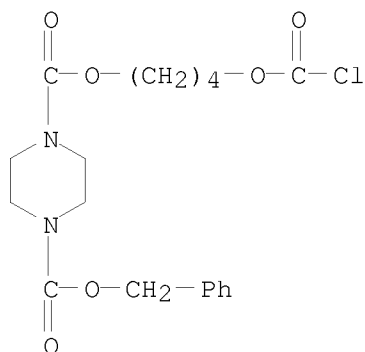
dicarboxylate

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and reaction of, with hexamethylene bis(piperazine-1-carboxylate))

RN 25539-29-1 CAPLUS

CN 1,4-Piperazinedicarboxylic acid, 4-[(chlorocarbonyl)oxy]butyl phenylmethyl ester (9CI) (CA INDEX NAME)



IT 124326-76-7P

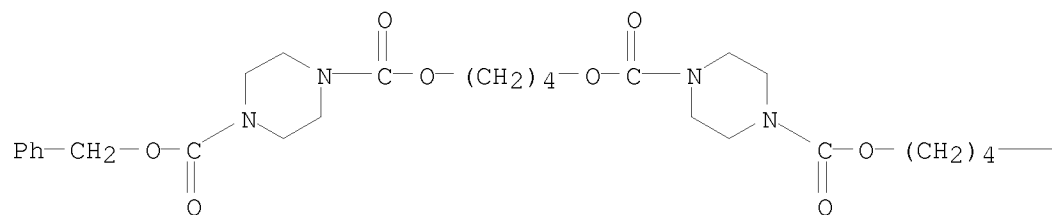
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and reaction of, with hexamethylene bis[[(piperazinylcarbonyloxy)butoxycarbonyl]piperazinecarboxylate] or

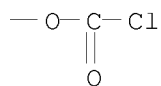
10/513699

hexamethylenebis[[(benzyloxycarbonyl)bis(piperazinediylcarbonyloxytetra
methylenecarbonyl)]piperazinecarboxylate])
RN 124326-76-7 CAPLUS
CN 1,4-Piperazinedicarboxylic acid, 4-[[[4-[[4-[(chlorocarbonyl)oxy]butoxy]ca
rbonyl]-1-piperazinyl]carbonyl]oxy]butyl phenylmethyl ester (9CI) (CA
INDEX NAME)

PAGE 1-A



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L4 ANSWER 14 OF 17 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1988:423523 CAPLUS
DOCUMENT NUMBER: 109:23523
TITLE: Preparation of nitrogen-containing bisphenols
INVENTOR(S): Shannon, Thomas Gerard; Brunelle, Daniel Joseph
PATENT ASSIGNEE(S): General Electric Co., USA
SOURCE: Ger. Offen., 12 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 3723610	A1	19880211	DE 1987-3723610	19870717 <--
US 4767877	A	19880830	US 1986-890054	19860728 <--
JP 63079863	A	19880409	JP 1987-183823	19870724 <--
PRIORITY APPLN. INFO.:			US 1986-890054	A 19860728

OTHER SOURCE(S): MARPAT 109:23523

AB The bisphenols Z1[(Z2)nCOZ3A2YA1OX]2 (A1, A2 = monocyclic arylene; X = H, COCl, COBr; Y = - or bridging group; Z1 = hydrocarbylene; Z2 = O or NR1; Z3 = NR2 when Z2 is O or n = 0, or O when Z2 = NR1 and n = 1 (R1 = H, hydrocarbyl; R3 = H, alkyl); n = 0 or 1] are useful in the preparation of cyclic heterocarbonates and linear polycarbonates. Thus, adding 25 mmol isophthaloyl chloride in 25 mL CH2Cl2 over 25 min to 50 mmol 4-HOC6H4C(Me)2C6H4NHMe-4, 50 mmol NaHCO3, 50 mL CH2Cl2, and 500 mL H2O stirred at high speed and stirring 10 min gave m-C6H4[CON(Me)p-C6H4C(Me)2C6H4OH-p]2 (I). Adding 1 g COCl2/min for 3 min to 6.12 g I in 50 mL CH2Cl2 at 0°, adding 3 g PhNEt2 in CH2Cl2 slowly at 0°, and stirring 15 min at room temperature gave a bis(chloroformate), polymerization of which in the presence of NaOH and Et3N gave a mixture (m.p. 140-160°) of polycarbonate-polyamide oligomers.

IT 114975-23-4P 114975-26-7P

RL: IMF (Industrial manufacture); PREP (Preparation)
(manufacture of, from cyclic oligomers)

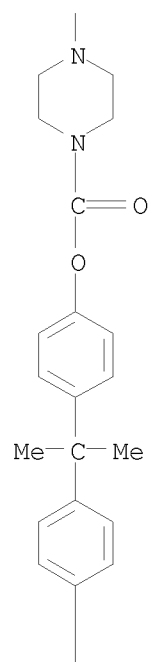
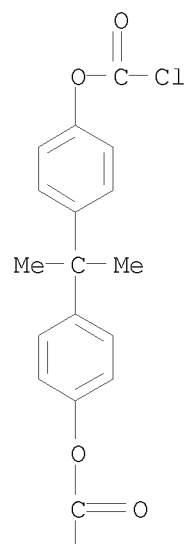
RN 114975-23-4 CAPLUS

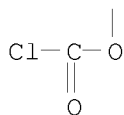
CN 1,4-Piperazinedicarboxylic acid, bis[4-[1-[4-[(chlorocarbonyl)oxy]phenyl]-1-methylethyl]phenyl] ester, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 114975-22-3

CMF C38 H36 Cl2 N2 O8





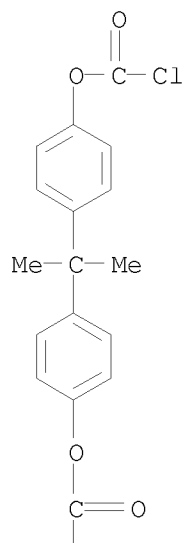
RN 114975-26-7 CAPLUS

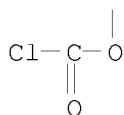
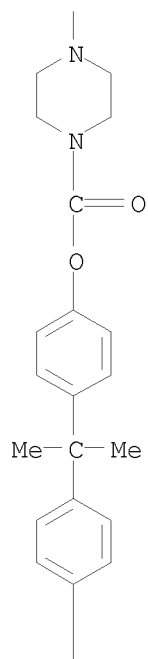
CN 1,4-Piperazinedicarboxylic acid, bis[4-[1-[4-[(chlorocarbonyl)oxy]phenyl]-1-methylethyl]phenyl] ester, polymer with (1-methylethylidene)di-4,1-phenylene bis(carbonochloridate) (9CI) (CA INDEX NAME)

CM 1

CRN 114975-22-3

CMF C38 H36 Cl2 N2 O8

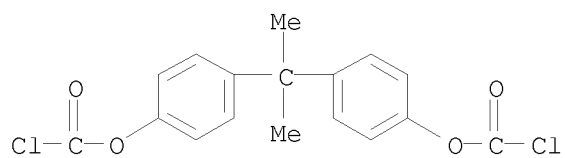




CM 2

CRN 2024-88-6

CMF C17 H14 C12 O4

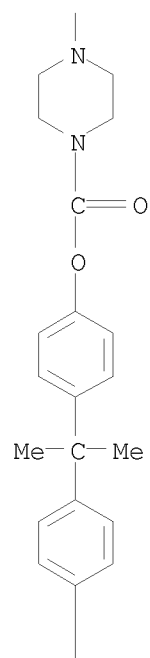
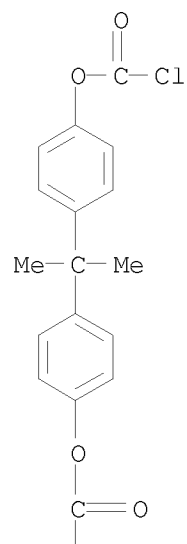


IT 114975-22-3P

RL: PREP (Preparation)
(preparation of)

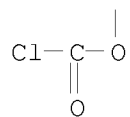
RN 114975-22-3 CAPLUS

CN 1,4-Piperazinedicarboxylic acid, bis[4-[1-[4-[(chlorocarbonyl)oxy]phenyl]-1-methylethyl]phenyl] ester (9CI) (CA INDEX NAME)



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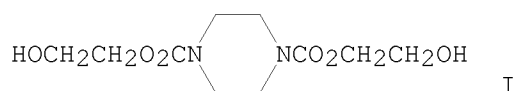


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L4 ANSWER 15 OF 17 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1976:543558 CAPLUS
DOCUMENT NUMBER: 85:143558
ORIGINAL REFERENCE NO.: 85:23021a,23024a
TITLE: Some copolyurethanes based on piperazine
AUTHOR(S): El-Giamal, Mohamed F.; Schulz, Rolf C.
CORPORATE SOURCE: Inst. Makromol. Chem., Tech. Hochsch. Darmstadt,
Darmstadt, Fed. Rep. Ger.
SOURCE: Makromolekulare Chemie (1976), 177(8),
2259-69
CODEN: MACEAK; ISSN: 0025-116X
DOCUMENT TYPE: Journal
LANGUAGE: German
GI

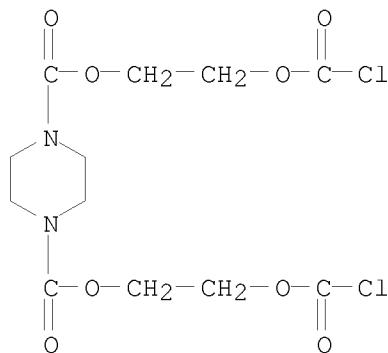


AB The diester I [7709-79-7] was prepared from piperazine [110-85-0] and ethylene carbonate [96-49-1]. I was copolymd. with aliphatic or aromatic dicarboxylic acid chlorides to prepare alternating polyesterurethanes. I was copolymd. with bis(4-isocyanatophenyl)methane to prepare a sequenced copolyurethane [60508-52-3]. Interfacial polycondensation of the bis(chloroformate) ester of I [60508-53-4] with aliphatic and aromatic diamines gave 6 ordered copolyurethanes.

IT 60508-53-4P 60508-54-5P 60508-55-6P
60508-56-7P 60508-57-8P 60508-58-9P
60508-59-0P 60508-60-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 60508-53-4 CAPLUS

CN 1,4-Piperazinedicarboxylic acid, bis[2-[(chlorocarbonyl)oxy]ethyl] ester
(9CI) (CA INDEX NAME)



RN 60508-54-5 CAPLUS

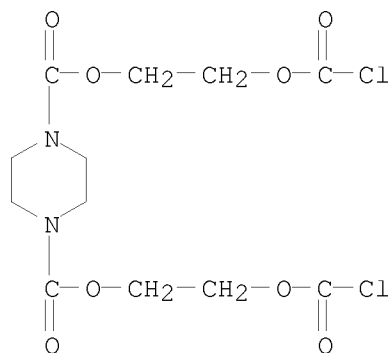
CN 1,4-Piperazinedicarboxylic acid, bis[2-[(chlorocarbonyl)oxy]ethyl] ester,
polymer with 1,3-benzenediamine (9CI) (CA INDEX NAME)

10/513699

CM 1

CRN 60508-53-4

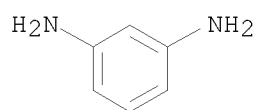
CMF C12 H16 C12 N2 O8



CM 2

CRN 108-45-2

CMF C6 H8 N2



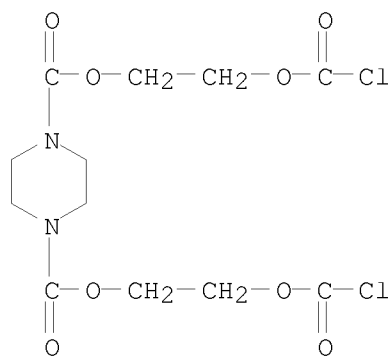
RN 60508-55-6 CAPLUS

CN 1,4-Piperazinedicarboxylic acid, bis[2-[(chlorocarbonyl)oxy]ethyl] ester, polymer with 1,4-benzenediamine (9CI) (CA INDEX NAME)

CM 1

CRN 60508-53-4

CMF C12 H16 C12 N2 O8



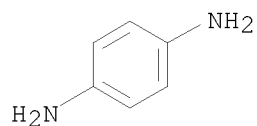
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10/513699

CM 2

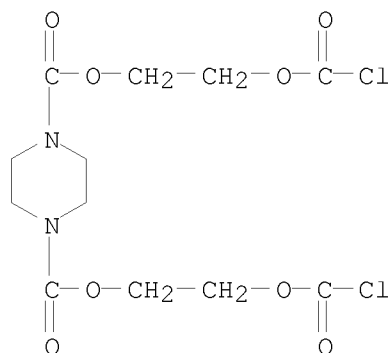
CRN 106-50-3
CMF C6 H8 N2



RN 60508-56-7 CAPLUS
CN 1,4-Piperazinedicarboxylic acid, bis[2-[(chlorocarbonyl)oxy]ethyl] ester,
polymer with 1,2-benzenediamine (9CI) (CA INDEX NAME)

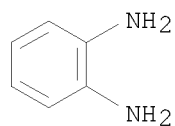
CM 1

CRN 60508-53-4
CMF C12 H16 Cl2 N2 O8



CM 2

CRN 95-54-5
CMF C6 H8 N2



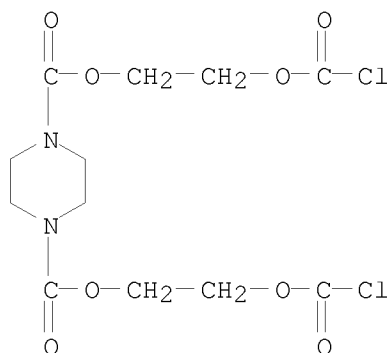
RN 60508-57-8 CAPLUS
CN 1,4-Piperazinedicarboxylic acid, bis[2-[(chlorocarbonyl)oxy]ethyl] ester,
polymer with 1,2-ethanediamine (9CI) (CA INDEX NAME)

CM 1

CRN 60508-53-4

10/513699

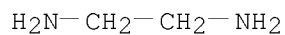
CMF C12 H16 C12 N2 O8



CM 2

CRN 107-15-3

CMF C2 H8 N2



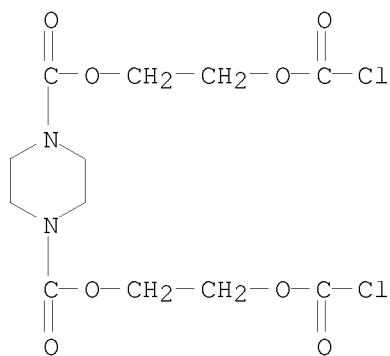
RN 60508-58-9 CAPLUS

CN 1,4-Piperazinedicarboxylic acid, bis[2-[(chlorocarbonyl)oxy]ethyl] ester, polymer with 1,6-hexanediamine (9CI) (CA INDEX NAME)

CM 1

CRN 60508-53-4

CMF C12 H16 C12 N2 O8



CM 2

CRN 124-09-4

CMF C6 H16 N2

<12/04/2007>

Erich Leese

10/513699

H₂N—(CH₂)₆—NH₂

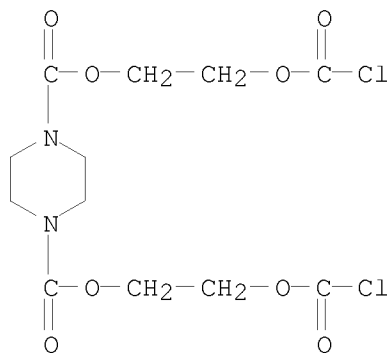
RN 60508-59-0 CAPLUS

CN 1,4-Piperazinedicarboxylic acid, bis[2-[(chlorocarbonyl)oxy]ethyl] ester,
polymer with 1,8-octanediamine (9CI) (CA INDEX NAME)

CM 1

CRN 60508-53-4

CMF C12 H16 C12 N2 O8



CM 2

CRN 373-44-4

CMF C8 H20 N2

H₂N—(CH₂)₈—NH₂

RN 60508-60-3 CAPLUS

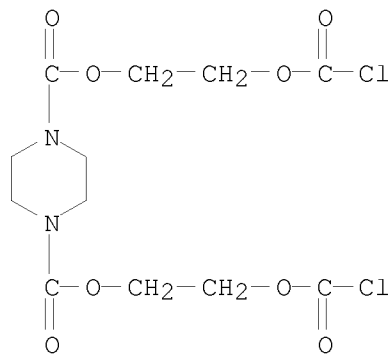
CN 1,4-Piperazinedicarboxylic acid, bis[2-[(chlorocarbonyl)oxy]ethyl] ester,
polymer with piperazine (9CI) (CA INDEX NAME)

CM 1

CRN 60508-53-4

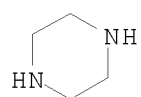
CMF C12 H16 C12 N2 O8

10/513699



CM 2

CRN 110-85-0
CMF C4 H10 N2



<12/04/2007>

Erich Leese

L4 ANSWER 16 OF 17 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1971:65438 CAPLUS
 DOCUMENT NUMBER: 74:65438
 ORIGINAL REFERENCE NO.: 74:10543a,10546a
 TITLE: Segmented polyurethanes containing monodisperse hard segments, useful as fibers and in making cast objects
 INVENTOR(S): Harrell, Leon L., Jr.
 PATENT ASSIGNEE(S): du Pont de Nemours, E. I., and Co.
 SOURCE: U.S., 6 pp.
 CODEN: USXXAM
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3541053	A	19701117	US 1968-748641	19680730 <--
JP 49006200	B	19740213	JP 1969-55548	19690715 <--
GB 1272072	A	19720426	GB 1969-1272072	19690730 <--
PRIORITY APPLN. INFO.:			US 1968-748641	A 19680730

GI For diagram(s), see printed CA Issue.

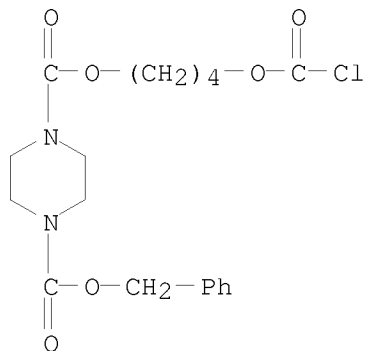
AB Segmented polyurethanes containing monodisperse hard segments derived from low-mol.-weight diols and diamines connected by urethane linkages to soft segments derived from polyether glycols were prepared Thus, copolymer (I) [preformed from piperazine, 1,4-butanediol, and benzyl chloroformate (and COCl₂) to a predetd. size (e.g., n = 2-12)] was dissolved in a CH₂Cl₂ solution of poly(tetramethylene ether) glycol (mol. weight 1000) bis(chloroformate). Aqueous Na₂CO₃ and a CH₂Cl₂ solution of 4,4-butyldienebis(3-methyl-6-tert-butylphenol) and 2,2-methylenebis(4-methyl-6-tert-butylphenol) were added, and the emulsion evaporated to give the polymer (II). These polymers had improved modulus, tensile strength and Shore A hardness.

IT 25539-29-1P

RL: IMF (Industrial manufacture); PREP (Preparation)
 (preparation of)

RN 25539-29-1 CAPLUS

CN 1,4-Piperazinedicarboxylic acid, 4-[(chlorocarbonyl)oxy]butyl phenylmethyl ester (9CI) (CA INDEX NAME)



10/513699

<12/04/2007>

Erich Leese

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ACCESSION NUMBER: 1970:32368 CAPLUS

DOCUMENT NUMBER: 72:32368

ORIGINAL REFERENCE NO.: 72:5957a,5960a

TITLE: Segmented polyurethanes. Properties as a function of segment size and distribution

AUTHOR(S): Harrell, L. L., Jr.

CORPORATE SOURCE: Exp. Sta., E. I. du Pont de Nemours and Co., Inc.,
Wilmington, DE, USA

SOURCE: Macromolecules (1969), 2(6), 607-12

CODEN: MAMOBX; ISSN: 0024-9297

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Property-structure relationships in a series of segmented polyurethanes were studied. The hard segment size, size distribution, and spacing along the chain (i.e., soft segment distribution) were varied independently by special synthetic techniques. The hard segments are crystalline and have well-defined m.p. which increase with segment size. Reciprocal absolute melting temperature is inversely proportional to the number of repeat units in the

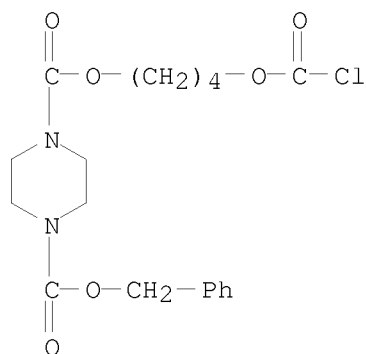
segment. Degree of crystallinity varies little with size. Cocrystn. of different hard segments is a function of relative size. Narrowing of the hard segment size distribution increases modulus, tensile, and extension set. Narrowing of the soft segment distribution causes increases in modulus, elongation, tensile, and extension set.

IT 25539-29-1P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 25539-29-1 CAPLUS

CN 1,4-Piperazinedicarboxylic acid, 4-[(chlorocarbonyl)oxy]butyl phenylmethyl ester (9CI) (CA INDEX NAME)



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Erich Leese